

# TRUE DIELECTRIC AND IDEAL CONDUCTOR IN THEORY OF THE DIELECTRIC FUNCTION FOR COULOMB SYSTEM

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On the basis of the exact relations the general formula for the static dielectric permittivity  $\varepsilon(q, 0)$  for Coulomb system is found in the region of small wave vectors  $q$ . The obtained formula describes the dielectric function  $\varepsilon(q, 0)$  of the Coulomb system in both states in the "metallic" state and in the "dielectric" one. The parameter which determines possible states of the Coulomb system - from the "true" dielectric till the "ideal" conductor is found. The exact relation for the pair correlation function for two-component system of electrons and nuclei  $g_{ec}(r)$  is found for the arbitrary thermodynamic parameters.

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## 1. Long wavelength dielectric function for Coulomb system: between dielectric and metallic states.

We consider the static dielectric permittivity  $\varepsilon(q, 0)$  for the homogeneous and isotropic Coulomb system. The function  $\varepsilon(q, 0)$  is determined as the proportionality coefficient between the potential  $U^{tot}(q, 0)$  of the total electric field in the medium and the external field potential  $U^{ext}(q, 0)$  [1]

$$U^{tot}(q, 0) = \frac{U^{ext}(q, 0)}{\varepsilon(q, 0)}. \quad (1)$$

According to [2,3] the function  $\varepsilon(q, 0)$  is connected with the static polarization operator  $\Pi(q, 0)$ , which determines the response of the system on the screened external field by the relation

$$\varepsilon(q, 0) = 1 - \frac{4\pi}{q^2} \Pi(q, 0), \quad (2)$$

$$\Pi(q, 0) = \sum_{a,b} z_a z_b e^2 \Pi_{ab}(q, 0), \quad (3)$$

where  $z_a e$ ,  $m_a$  and  $n_a$  are the charge, the mass and the average density of the particles of the sort  $a$  in the system with the chemical potentials  $\mu_a$  at temperature  $T$ . The system is considered under the condition of quasineutrality

$$\sum_a e z_a n_a = 0 \quad (4)$$

The functions  $\Pi_{ab}(q, 0)$  are the partial polarization operators of the particle species  $a$  and  $b$ . In diagram technique [2,3] the functions  $\Pi_{ab}(q, 0)$  are the irreducible (on one-line of the Coulomb interaction in the  $q$ -channel) parts of the appropriate "density-density" Green functions  $\chi_{ab}(q, 0)$ , which determine response of the system on an external field. In contrast with the Green functions  $\chi_{ab}(q, 0)$  of the Coulomb systems, the polarization functions  $\Pi_{ab}(q, 0)$  do not consist the singularities and are the smooth functions in the region of small wave vectors  $q$  (at least for the normal systems). Therefore, the functions  $\Pi_{ab}(q, 0)$  for the small values of  $q$  can be represented in the form

$$\Pi_{ab}(q, 0) \simeq \pi_{ab}^{(0)} + q^2 \pi_{ab}^{(2)}, \quad (5)$$

$$\pi_{ab}^{(0)} = \lim_{q \rightarrow 0} \Pi_{ab}(q, 0), \quad \pi_{ab}^{(2)} = \lim_{q \rightarrow 0} \left[ \frac{\Pi_{ab}(q, 0) - \lim_{q \rightarrow 0} \Pi_{ab}(q, 0)}{q^2} \right]. \quad (6)$$

In [4,5] it was shown that

$$\pi_{ab}^{(0)} = - \left( \frac{\partial n_a}{\partial \mu_b} \right)_T. \quad (7)$$

Eq. (7) is the generalization for the many-component Coulomb system the well known result for the model case of the one-component electron liquid, where this kind of equality is called "the sum rule for compressibility"[6]

$$\pi_{ee}^{(0)} = - \left( \frac{\partial n_e}{\partial \mu_e} \right)_T = -n_e^2 K_T^e, \quad K_T = -\frac{1}{V} \left( \frac{\partial V}{\partial P} \right)_T, \quad (8)$$

where  $V$ ,  $P$  and  $K_T$  are respectively the volume, pressure and the isothermal compressibility of the Coulomb system. In one's turn, for the two-component Coulomb system which consists the electrons (index -  $e$ ) and nuclei (index -  $c$ ), the limiting relations [4,5] for the static structure factors  $S_{ab}(q)$  can be found on the basis of Eq. (8)

$$\lim S_{cc}(q \rightarrow 0) = n_c T K_T; \quad \lim S_{cc}(q \rightarrow 0) = \frac{n_c}{n_e} \lim S_{ee}(q \rightarrow 0) = \left( \frac{n_c}{n_e} \right)^{1/2} \lim S_{ec}(q \rightarrow 0) \quad (9)$$

The functions  $S_{ab}(q)$  are measured directly, including the critical point region [7], in the experiments on the neutron scattering. By inserting (5), (6) in (2) and (3) we obtain in the long-wavelength limit (the small values of  $q$ ) for the dielectric function of the Coulomb system of an arbitrary composition the following relations

$$\varepsilon(q, 0) = \varepsilon_0^{st} + \frac{\kappa^2}{q^2}, \quad \kappa^2 = -4\pi \sum_{ab} e^2 z_a z_b \pi_{ab}^{(0)} = 4\pi \sum_{ab} e^2 z_a z_b \left( \frac{\partial n_a}{\partial \mu_b} \right)_T \quad (10)$$

$$\varepsilon_0^{st} = 1 + 4\pi\alpha, \quad \alpha = - \sum_{ab} e^2 z_a z_b \pi_{ab}^{(2)} \quad (11)$$

It is evident, that all the coefficients in Eqs. (10), (11) are the functions of the thermodynamic parameters of the Coulomb system. By use of the grand canonical ensemble one easily arrive [8] at the equality

$$T \left( \frac{\partial n_a}{\partial \mu_b} \right)_T = \frac{1}{V} \langle \delta N_a \delta N_b \rangle, \quad \delta N_a = N_a - \langle N_a \rangle, \quad (12)$$

where  $n_a = \langle N_a \rangle / V$ ,  $N_a$  is the operator of the total number of particles of the sort  $a$  and the brackets  $\langle \dots \rangle$  means the averaging on the grand canonical ensemble.

Inserting (12) in (10) and taking into account the quasineutrality condition we find for the Coulomb system at the arbitrary parameters

$$\kappa^2 = \frac{4\pi}{T} \frac{\langle Z^2 \rangle}{V} \geq 0, \quad Z = \sum_a z_a e N_a. \quad (13)$$

We have mention that the sign of the value  $\alpha$  which is introduced by Eq. (11) is not determined in the moment. It is easy to see from (11) that the value  $\kappa$  coincides in the appropriate limiting cases with the Debye and the Thomas-Fermi wave vectors (see, e.g., [3]).

As an illustration, let us consider the action of the point charge on the infinite homogeneous Coulomb system. Then, taking into account (1), in  $r$ -space we obtain

$$\frac{U^{tot}(r)}{U^{ext}(r)} = \frac{2}{\pi} \int_0^\infty \frac{dq}{q} \frac{\sin(qr)}{\varepsilon(q, 0)} \quad (14)$$

In the limit  $r \rightarrow \infty$  from Eqs. (10), (14) directly follows

$$\frac{U^{tot}(r)}{U^{ext}(r)} \rightarrow \frac{1}{\varepsilon_0^{st}} \exp(-r/R_{scr}), \quad R_{scr} = \left( \frac{\varepsilon_0^{st}}{\kappa^2} \right)^{1/2}, \quad (15)$$

where  $R_{scr}$  is the electrostatic field penetration length in matter, or the screening radius, according to the terminology, accepted in the theory of non-ideal plasma (see, e.g., [9]). This value, as it follows from (10), characterizes the depth of penetration for the electromagnetic field in the medium.

In the limiting case

$$\frac{4\pi}{TV} \langle Z^2 \rangle \rightarrow 0, \quad \kappa^2 \rightarrow 0 \quad (16)$$

the screening radius  $R_{scr}$  tends to infinity

$$R_{scr} \rightarrow \infty \quad (17)$$

Therefore, when the condition (16) is fulfilled, the Coulomb system manifests itself as an "true" dielectric, which changes only the amplitude of the electrostatic field on the value  $\varepsilon_0^{st}$  (11). In this sense the value  $\varepsilon_0^{st}$  can be treated as the dielectric constant of the medium. Accordingly, the value  $\alpha$  in (11) can be considered as the electric polarization of the medium.

It is necessary to stress the essential circumstance. As in the case of "traditional" consideration of the "metal-dielectric" transition on basis of the analysis of the electron conductivity (see, e.g., [10],[11]), one can maintain the relative character of the division of matter on dielectrics and conductors, since all dielectrics possess the non-zero conductivity for  $T \neq 0$ . The similar statement is applied to the depth of penetration  $R_{scr}$  (15) of the electrostatic field in matter. In metals the penetration depth is very small in contrast with dielectrics, where it can be of one order with the size of the system.

The indirect confirmation of this statement contains in [3], where the generalized random phase approximation for calculation of the polarization function  $\Pi(q, 0)$  is developed. This approximation permits to take into account the bounded states of the electrons and nuclei. In fact, it means the possibility to separate the states in the Coulomb systems on "localized" and "delocalized" ones. In the last case the charged particles can spread on the whole volume of the considering system.

In the opposite to (16) limiting case

$$\frac{4\pi}{TV} < Z^2 > \rightarrow \infty, \quad \kappa^2 \rightarrow \infty, \quad (18)$$

$$R_{scr} \rightarrow 0. \quad (19)$$

If in the respective thermodynamic state the penetration length  $R_{scr}$  for the electrostatic field tends to zero the system can be treated not simply as in the "metallic" state but as an "ideal" conductor. In this limiting case the electrostatic field cannot penetrate in the matter at all (in the limiting interpretation, naturally).

Meanwhile the question arises on the relation between the true "dielectric" and "ideal" conductor from one side and the static conductivity  $\sigma_{st}$  for the Coulomb system. In this connection we have notice that according to the perturbation theory of the diagram technique for Coulomb systems [2,3] the charged particles interact by the screening Coulomb potential  $U_{ab}^{scr}$

$$U_{ab}^{scr}(q) = \frac{4\pi z_a z_b e^2}{q^2 \varepsilon(q, 0)}, \quad (20)$$

which is similar to (1).

In the case when the limiting conditions (16) are fulfilled the interaction potential  $U_{ab}^{scr}(q)$  for small  $q$  (or for large distances) is similar to the initial Coulomb potential. Therefore, one can suggest that the charged particles form the collective "localized" state with the conductivity  $\sigma_{st}$  equals to zero.

In the opposite limiting case (18) the initial Coulomb potential is suppressed and one can suggest that the charged particles are in the fully "delocalized" state with the conductivity  $\sigma_{st}$  tends to infinity.

Therefore, we can assert, that the representation of the dielectric permittivity  $\varepsilon(q, 0)$  in the region of small wave vectors  $q$  in the form Eq. (10) is universal and can be used for description of the Coulomb system in both, the "metallic" and the "dielectric" states of matter. The parameter  $< Z^2 > / V$ , changing from 0 to  $\infty$ , determines the variety of the states of the Coulomb system - from the state of the "true" dielectric and till the state of the "ideal" conductor.

2. The analysis performed above is referred to the Coulomb systems with two or more components of charged particles and to strong inter-particle interaction. Since theoretical description of these systems is difficult, the exact relations for the correlation functions of such systems are very important and useful.

According to Eqs. (2),(3),(10),(13) for the small values of wave vectors  $q$  for the static dielectric function  $\varepsilon(q, 0)$  the inequality

$$\varepsilon(q, 0) > 1, \quad (21)$$

is fulfilled.

As shown in [12-14] from the inequality (21) follows, that the dielectric permittivity  $\varepsilon(q, \omega)$  satisfies to the Kramers-Kronig relations

$$Re\varepsilon(q, \omega) = 1 + P \int_{-\infty}^{\infty} \frac{Im\varepsilon(q, \xi)}{\pi} \frac{d\xi}{\xi - \omega}, \quad (22)$$

$$Im\varepsilon(q, \omega) = -P \int_{-\infty}^{\infty} \frac{Re\varepsilon(q, \xi) - 1}{\pi} \frac{d\xi}{\xi - \omega}. \quad (23)$$

Symbol  $P$  means that we consider the main value of the integral. From (22) taking into account the relations [6]:

$$Re\varepsilon(q, \omega) = Re\varepsilon(q, -\omega), \quad Im\varepsilon(q, \omega) = -Im\varepsilon(q, -\omega) \quad (24)$$

$$Im\varepsilon(q, \omega) > 0 \quad \text{for } \omega > 0 \quad (25)$$

is easy to see [15] that for the moments  $m_n(q)$  of the high-frequency ( $\omega \rightarrow \infty$ ) expansion of the function  $Re\varepsilon(q, \omega)$

$$Re\varepsilon(q, \omega) = 1 - \sum_{n=1}^{\infty} \frac{m_n(q)}{\omega^{2n}}, \quad (26)$$

is fulfilled the condition

$$m_n(q) = \frac{2}{\pi} \int_0^{\infty} \xi^{2n} Im\varepsilon(q, \xi) d\xi. \quad (27)$$

According to the given above consideration the inequality (27) is true in the long wavelength limit ( $q \rightarrow 0$ ) for an arbitrary thermodynamic parameters in homogeneous and isotropic Coulomb system.

Let us use for further consideration the expressions for two first momenta  $m_1(q)$  and  $m_2(q)$  [16,17]

$$m_1(q) = \omega_p^2, \quad (28)$$

$$\begin{aligned} m_2(q) = & \sum_a \omega_a^2 \left\{ \frac{2T_a q^2}{m_a} + \frac{\hbar^2 q^4}{4m_a^2} \right\} + \sum_{a,b} (n_a n_b)^{1/2} \int_0^{\infty} k^2 (S_{ab}(k) - \delta_{a,b}) \\ & \times \left\{ \frac{z_a^2 z_b^2 e^4}{m_a m_b} \left[ \frac{(q^2 - k^2)^2}{k q^3} \ln \left| \frac{q+k}{q-k} \right| - \frac{2k^2}{q^2} + 6 \right] - \frac{8z_a^3 z_b e^4}{3m_a^2} \right\} dk, \end{aligned} \quad (29)$$

Here  $T_a$  is the exact average kinetic energy referred to one particle of the sort  $a$ ,  $S_{a,b}(q)$  - the static structure factor for the particles of the species  $a$  and  $b$ , which is connected with the pair correlation function  $g_{a,b}(r)$ ,

$$S_{ab}(q) = \delta_{a,b} + (n_a n_b)^{1/2} \int \exp(i\mathbf{qr}) \{g_{ab}(r) - 1\} d\mathbf{r} \quad (30)$$

$\omega_p$  is the plasma frequency of the Coulomb system,  $\omega_a$  is the plasma frequency of the charges of the sort  $a$

$$\omega_a = \left( \frac{4\pi z_a^2 e^2 n_a}{m_a} \right)^{1/2}, \quad \omega_p = \left( \sum_a \omega_a^2 \right)^{1/2}. \quad (31)$$

For derivation of the relation (29) we used the potentials of the Coulomb inter-particle interaction

$$u_{ab}(q) = \frac{4\pi z_a z_b e^2}{q^2}. \quad (32)$$

From (29) follows [15]

$$m_2(0) = \lim_{q \rightarrow 0} m_2(q) = \frac{8}{3} \sum_{a,b} (n_a n_b)^{1/2} \left\{ \frac{z_a^2 z_b^2 e^4}{m_a m_b} - \frac{z_a^3 z_b e^4}{m_a^2} \right\} \int_0^{\infty} k^2 S_{ab}(k) dk \quad (33)$$

In the particular case of the two-component Coulomb system, consisting the electrons (index  $e$ ) and nuclei (index  $c$ ), from (33) under the quasi neutrality condition (4) we arrive at the expression

$$m_2(0) = \frac{\omega_e^4}{3} \left( 1 + \frac{z_c m_e}{m_c} \right) \{g_{ec}(0) - 1\} \quad (34)$$

Therefore, according to (27) in the homogeneous and isotropic two-component Coulomb system the inequality

$$g_{ec}(0) \geq 1 \quad (35)$$

has to be fulfilled for the arbitrary thermodynamic parameters.

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